CAS ONLINE PRINTOUT

STN Search
by Prim Examiner SBarts
9/11/07

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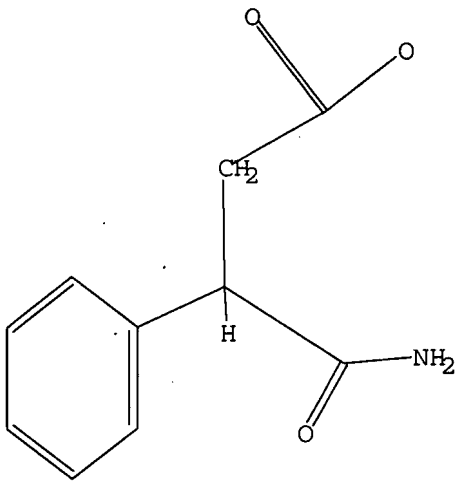

Structure attributes must be viewed using STN Express query preparation.

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=> d bib abs hitstr 1-24

L17  ANSWER 1 OF 24  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2007:332826  CAPLUS
DN   146:358579
TI   Preparation of conformationally constrained 3-(4-hydroxyphenyl)-
     substituted propanoic acids useful for treating metabolic disorders
IN   Akerman, Michelle; Brown, Sean; Houze, Jonathan B.; Liu, Jinqian; Ma,
     Zhihua; Medina, Julio C.; Qiu, Wei; Schmitt, Michael J.; Wang, Yingcai;
     Zhu, Liusheng
PA   Amgen Inc., USA
SO   PCT Int. Appl., 228pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.          DATE
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PI   WO 2007033002        A1    20070322    WO 2006-US34995          20060908
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP,
             KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN,
             MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,
             RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
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         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PI US 2007066647 A1 20070322 US 2006-517992 20060908

PRAI US 2005-717432P P 20050914

OS MARPAT 146:358579

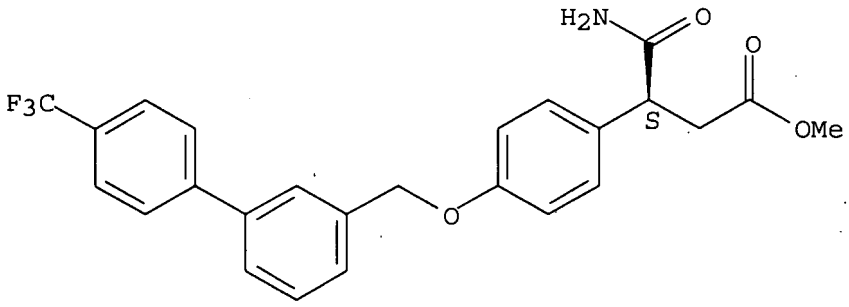
AB QL1PL2MXL3A [Q = H, aryl, heteroaryl, alkyl, heteroalkyl; L1 = bond, alkylene, heteroalkylene, O, S, SO, SO2, NRa, carbonylheterocycloalkylene, alkylenesulfonylamino, alkyleneaminosulfonyl, carbonylamino; P = cyclohexyl, benzocycloalkyl; L2 = bond, alkylene, heteroalkylene, oxymethylene, O, S, SO, SO2, NRa, alkylenesulfonylamino, etc.; M = aryl, heteroaryl, cycloalkyl, arylalkylene, heteroarylalkylene; X = CR1R11, NR1, O, S, SO, SO2; L3 = alkylene, heteroalkylene; A = CO2H, tetrazol-5-yl, SO3H, PO3H2, CONHSO2Me, CHO, thiazolidinedionyl, hydroxyphenyl, pyridyl; Ra = H, alkyl, aralkyl, heteroalkyl; R1 = cyano, aryl, heteroaryl, alkenyl, alkynyl, carboxamide; R11 = H, cyano, aryl, heteroaryl, alkyl, alkenyl, alkynyl], were prepared Thus, (3S)-3-[4-[5-(3-trifluoromethylphenyl)-2,3-dihydro-1H-inden-1-yloxy]phenyl]hex-4-ynoic acid [preparation from 5-bromo-1-indanone, Me (S)-3-(4-hydroxyphenyl)hex-4-ynoate, and 4-trifluoromethylboronic acid given] showed an EC50 of <0.01 μM in a cell-based aequorin assay for relative activation of GPR40.

IT 916219-96-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of conformationally constrained hydroxyphenylpropanoates for treating metabolic disorders)

RN 916219-96-0 CAPLUS

CN Benzenepropanoic acid, β-(aminocarbonyl)-4-[[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]methoxy]-, methyl ester, (βS)- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:1256706 CAPLUS

DN 146:27822

TI Preparation of benzyloxyphenyl(azolyl)alkanoates as modulators of G-protein coupled receptor GPR40 for treatment of metabolic disorders.

IN Houze, Jonathan; Liu, Jiwen; Ma, Zhihua; Medina, Julio C.; Schmitt, Michael J.; Sharma, Rajiv; Sun, Ying; Wang, Yingcai; Zhu, Liusheng

PA Amgen Inc., USA

SO PCT Int. Appl., 88pp.
CODEN: PIXXD2

DT Patent

LA English

CAS ONLINE PRINTOUT

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006127503	A2	20061130	WO 2006-US19545	20060518
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	US 2006270724	A1	20061130	US 2006-436732	20060517
PRAI	US 2005-683331P	P	20050520		
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OS MARPAT 146:27822

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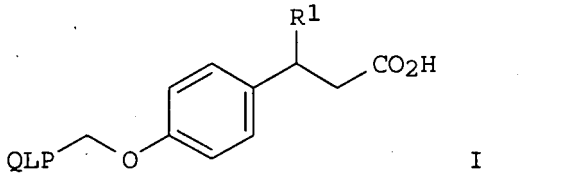

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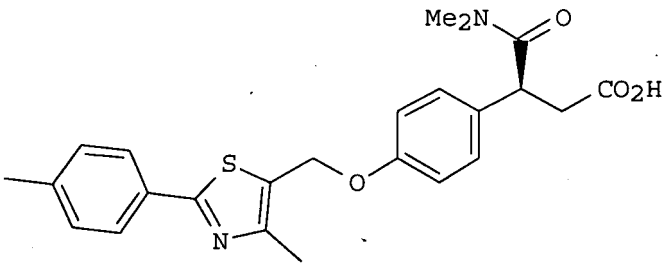


I

AB Title compds. [I; Q = (substituted) Ph; L = bond, O; P = phenylene, (substituted) thiazolylene; R1 = (substituted) oxazolyl, imidazolyl, triazolyl, tetrazolyl, carboxamide], were prepared Thus, title compound (II) (prepared via coupling of the corresponding thiazolyl chloride and phenol derivs.) showed an EC50 <0.01 μM in a cell based aequorin assay for modulatory activity on the GPR40 signaling pathway.

IT 916219-96-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

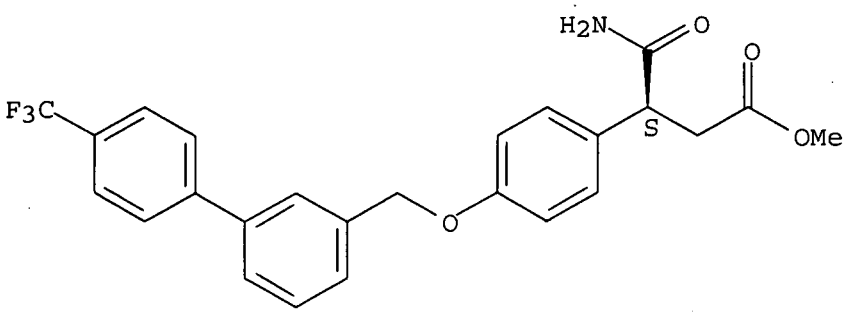
(preparation of benzyloxyphenyl(azolyl)alkanoates as modulators of GPR40 for treatment of metabolic disorders)

RN 916219-96-0 CAPLUS

CN Benzenepropanoic acid, β-(aminocarbonyl)-4-[[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]methoxy]-, methyl ester, (βS)- (CA INDEX NAME)

CAS ONLINE PRINTOUT

Absolute stereochemistry.



L17 ANSWER 3 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1026833 CAPLUS
DN 143:326090
TI Preparation of arylmethoxyphenyl-alkylcarboxylic acids and related derivatives for use in treating metabolic disorders
IN Akerman, Michelle; Houze, Jonathan; Lin, Daniel C. H.; Liu, Jiwen; Luo, Jian; Medina, Julio C.; Qiu, Wei; Reagan, Jeffrey D.; Sharma, Rajiv; Shuttleworth, Stephen J.; Sun, Ying; Zhang, Jian; Zhu, Liusheng
PA Amgen Inc., USA; et al.
SO PCT Int. Appl., 163 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005086661	A2	20050922	WO 2005-US5815	20050224
	WO 2005086661	A3	20060504		
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	AU 2005220728	A1	20050922		
	CA 2558585	A1	20050922	CA 2005-2558585	20050224
	EP 1737809	A2	20070103	EP 2005-723623	20050224
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	BR 2005008098	A	20070717	BR 2005-8098	20050224
	JP 2007525516	T	20070906	JP 2007-500959	20050224
	US 2006004012	A1	20060105	US 2005-67377	20050225
	MX 2006PA09793	A	20061030	MX 2006-PA9793	20060828
	US 2007142384	A1	20070621	US 2006-591214	20060828
	IN 2006DN05525	A	20070817	IN 2006-DN5525	20060922
	NO 2006004362	A	20061122	NO 2006-4362	20060926
PRAI	US 2004-548741P	P	20040227		
	US 2004-601579P	P	20040812		

CAS ONLINE PRINTOUT

WO 2005-US5815 W 20050224
OS MARPAT 143:326090
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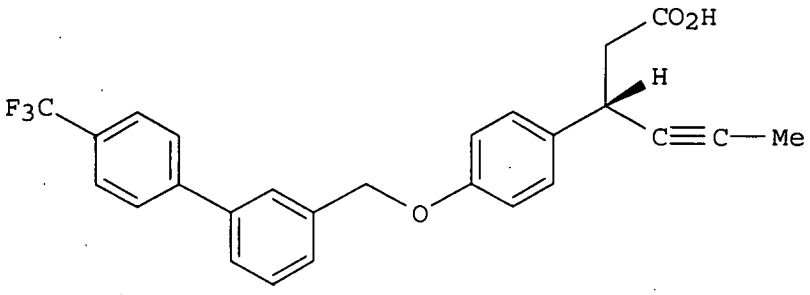
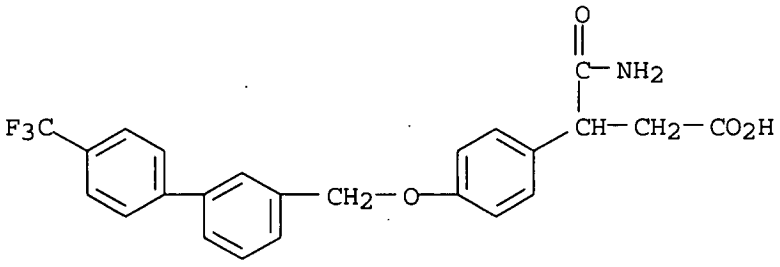


II

AB Title compds. Q-L1-P-L2-M-X-L3-A [Q = H, (hetero)aryl, alkyl, etc.; L1 = bond, alkylene, heteroalkylene, O, etc.; P = (hetero)aromatic, cycloalkylene, etc.; L2 = bond, alkylene, heteroalkylene, etc.; M = (hetero)aromatic, cycloalkylene, arylalkylene, etc.; X = divalent alkyl, (un)substituted-N; O, SO0-2; L3 = bond, alkylene, heteroalkylene, etc.; A = COOH, tetrazolyl, SO3H, PO3H2, etc.; I] are prepared For instance, (S)-3-[4-((4'-trifluoromethyl-1,1'-biphenyl-3-yl)methoxy)phenyl]hexan-4-ynoic acid (II) is prepared in 5 steps from (S)-3-(4-hydroxyphenyl)hexan-4-ynoic acid Me ester (preparation given), 4-(trifluoromethyl)phenylboronic acid and 3-bromobenzoic acid. II has an EC50 < 0.1 μM for human G protein-coupled receptor GPR40. I are useful for the treatment of type II diabetes.

IT 865233-31-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylmethoxyphenyl-alkylcarboxylic acids and related derivs. as GPCR40 ligands for use in treating metabolic disorders)

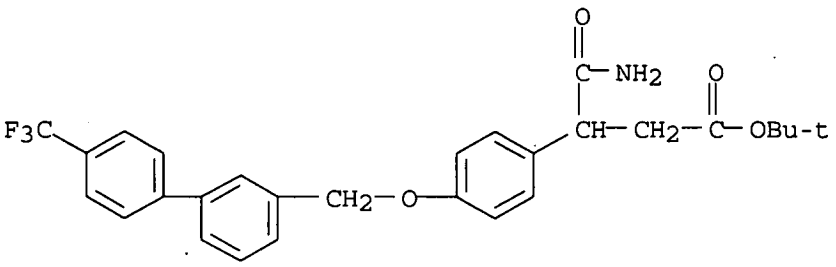
RN 865233-31-4 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-[[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]methoxy]- (9CI) (CA INDEX NAME)



IT 865233-79-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylmethoxyphenyl-alkylcarboxylic acids and related derivs. as GPCR40 ligands for use in treating metabolic disorders)

RN 865233-79-0 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-[[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]methoxy]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT



L17 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:158625 CAPLUS
DN 142:261292
TI Preparation of (hetero)aryl-substituted succinate derivatives as matrix metalloproteinase inhibitors
IN Holmes, Ian; Watson, Stephen Paul
PA Glaxo Group Limited, UK
SO PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005016868	A2	20050224	WO 2004-EP9087	20040812
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	US 2006235074	A1	20061019	US 2006-569812	20060210
PRAI	GB 2003-19069	A	20030814		
	WO 2004-EP9087	W	20040812		

OS CASREACT 142:261292; MARPAT 142:261292
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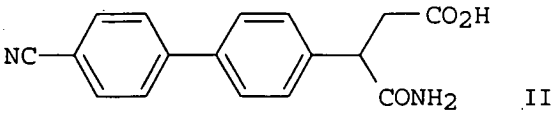


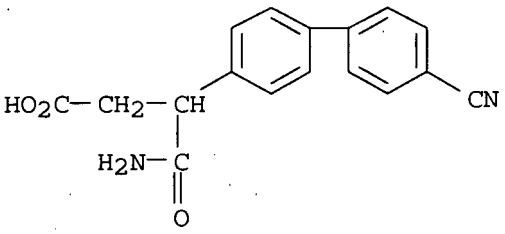
II

AB Title compds. represented by the formula I, R1ZQCH(R2)CH2X, [wherein R1 = (un)substituted alkyl(cycloalkyl), alkylheterocycloalkyl, alkylaryl, etc.;

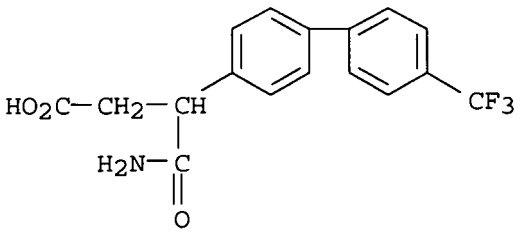
Z = a bond, CH2, O, S, etc.; Q = (un)substituted (hetero)aryl; X = COR3; R2 = CONH2, CO2H, sulfonylamino, etc.; R3 = OH, oxyalkyl or (un)substituted amino; with a proviso; and physiol. functional derivs. thereof] were prepared as matrix metalloproteinase (MMP) inhibitors. Coupling reaction of 4-amino-3-(4-bromophenyl)-4-oxobutanoic acid with p-nitrilephenylboronic acid gave II in 100% yield. I showed inhibition of MMP-12 with IC50 values of below 100 μM. Thus, I and their pharmaceutical compns. are useful as matrix metalloproteinase inhibitors for the treatment of inflammation or autoimmune disease (no data).

IT 845786-15-4P 845786-16-5P 845786-17-6P
845786-18-7P 845786-19-8P 845786-20-1P
845786-21-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (hetero)aryl-substituted succinate derivs. as matrix metalloproteinase inhibitors)

RN 845786-15-4 CAPLUS
CN [1,1'-Biphenyl]-4-propanoic acid, β-(aminocarbonyl)-4'-cyano- (9CI) (CA INDEX NAME)



RN 845786-16-5 CAPLUS
CN [1,1'-Biphenyl]-4-propanoic acid, β-(aminocarbonyl)-4'-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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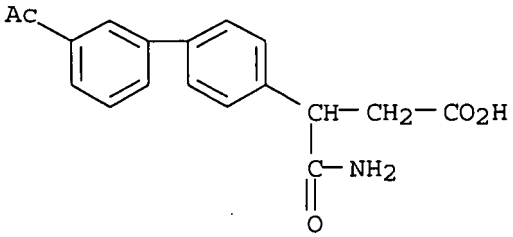
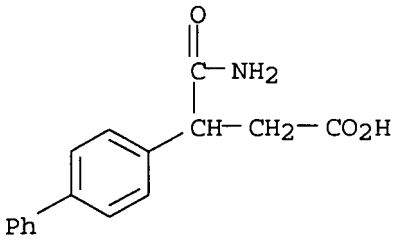


CAS ONLINE PRINTOUT

RN 845786-18-7 CAPLUS
CN [1,1'-Biphenyl]-4-propanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



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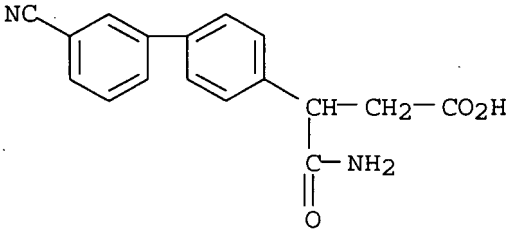

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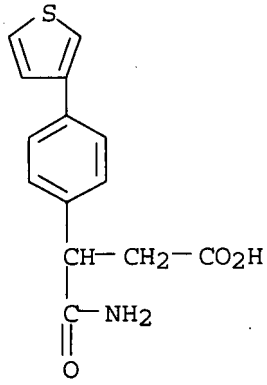
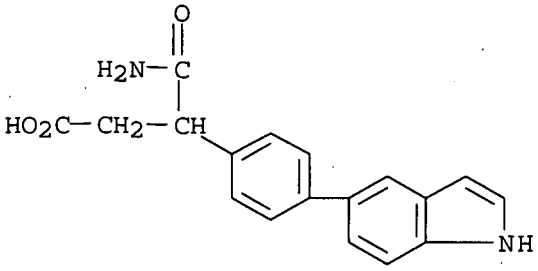
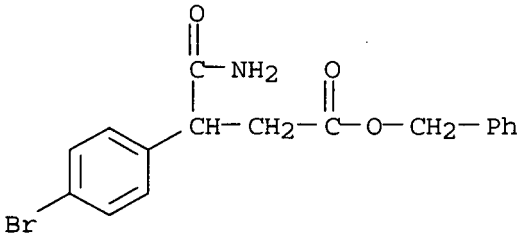


RN 845786-21-2 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-(1H-indol-5-yl)- (9CI) (CA INDEX NAME)

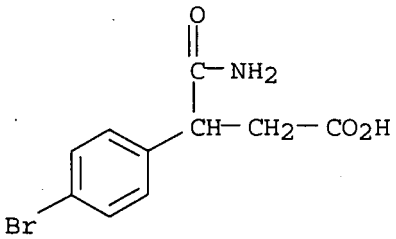
CAS ONLINE PRINTOUT



IT 845785-99-1P 845786-00-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (hetero)aryl-substituted succinate derivs. as matrix metalloproteinase inhibitors)
RN 845785-99-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-bromo-, phenylmethyl ester (9CI) (CA INDEX NAME)

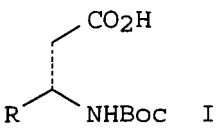


RN 845786-00-7 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-bromo- (9CI) (CA INDEX NAME)

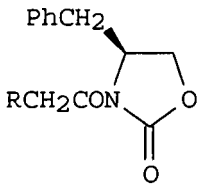


L17 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:960925 CAPLUS
DN 138:321520
TI A convenient synthesis of chiral β3-amino acids
AU Chakraborty, Tushar K.; Ghosh, Animesh
CS Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SO Synlett (2002), (12), 2039-2040
CODEN: SYNLES; ISSN: 0936-5214
PB Georg Thieme Verlag
DT Journal
LA English
OS CASREACT 138:321520
GI

CAS ONLINE PRINTOUT



I



II

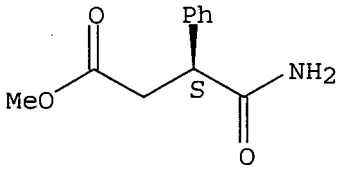
AB A novel method for the synthesis of chiral β3-amino acids is developed where the acid functionality was built by oxidative cleavage of an α-allylic group that was introduced by Evans' asym. alkylation of an appropriate acid substrate and the amino part came from the amide of the original carboxyl group following a modified Hofmann rearrangement reaction. Thus, amino acids I (R = Ph, Me, CHMe2, C8H17, C16H33) were prepared in six steps from starting material oxazolidinones II.

IT 511550-50-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral β-amino acids from (benzyl)oxazolidinone derivs.)

RN 511550-50-8 CAPLUS

CN Benzenepropanoic acid, β-(aminocarbonyl)-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 6 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1988:486102 CAPLUS

DN 109:86102

TI Succinimide derivatives: chemical structure-anticonvulsant activity relation

AU Avetisyan, S. A.; Nesunts, N. S.; Buyukyan, N. S.; Mndzhoyan, O. L.; Dzhagatspanyan, I. A.; Nazaryan, I. M.; Akopyan, N. E.

CS Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR

SO Khimiko-Farmatsevticheskii Zhurnal (1988), 22(4), 433-8
CODEN: KHFZAN; ISSN: 0023-1134

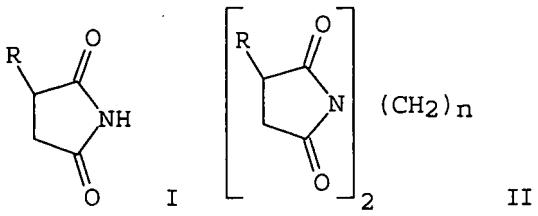
DT Journal

LA Russian

OS CASREACT 109:86102

GI

CAS ONLINE PRINTOUT



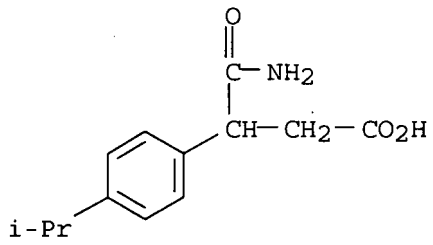
I II

AB Succinimides (I, R = 4-isopropylphenyl, or 4-cyclopropylphenyl) were prepared by the conversion of the corresponding benzyl chlorides to aldehydes, Knoevenagel reaction with di-Et malonate, HCN addition to the resulting ylidene malonates, hydrolysis, amidation-hydrolysis and cyclization. Treatment of I (R = 4-isopropoxyphenyl) with N2H4 gave N,N'-bis(p-isopropoxyphenylsuccinimide) (II, R = p-isopropoxyphenyl, n = 0). Similarly, other II (R = p-isopropoxyphenyl and n = 1-10) were prepared Of all the compds. studied, I (R = 4-isopropylphenyl, or 4-cyclopropylphenyl) and II (R = 4-isopropoxyphenyl and n = 0, 1, 2, 3, or 4) were completely devoid of the ability to prevent nicotinic hyperkinesis and arecoline tremors, as shown in mice. However, I and pufamide showed anticonvulsant activity in relation to corazole and elec. shock. Antagonism to corazole was observed in 50% of the animals at 68 and 90 mg/kg for I (R = 4-isopropylphenyl and 4-cyclopropylphenyl), resp., and to elec. shock at doses 92 and 94 mg/kg. Structure-activity relations are discussed.

IT 115906-13-3P 115906-14-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

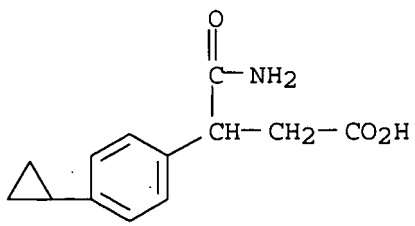
RN 115906-13-3 CAPLUS

CN Benzenepropanoic acid, β-(aminocarbonyl)-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



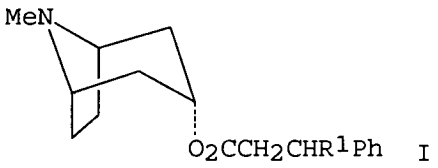
RN 115906-14-4 CAPLUS

CN Benzenepropanoic acid, β-(aminocarbonyl)-4-cyclopropyl- (9CI) (CA INDEX NAME)



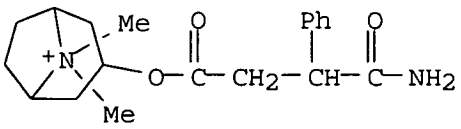
CAS ONLINE PRINTOUT

L17 ANSWER 7 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1988:406374 CAPLUS
DN 109:6374
TI Synthesis and anticholinergic activity of 8-methyl-8-azabicyclo[3.2.1]octane analogs of atropine
AU Amin, K. M.; Hassan, A. B.
CS Fac. Pharm., Cairo Univ., Egypt
SO Egyptian Journal of Pharmaceutical Sciences (1987), 28(1-4), 149-61
CODEN: EJPSBZ; ISSN: 0301-5068
DT Journal
LA English
OS CASREACT 109:6374
GI

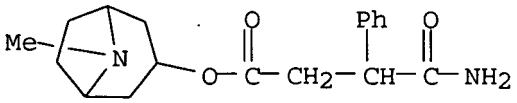


I

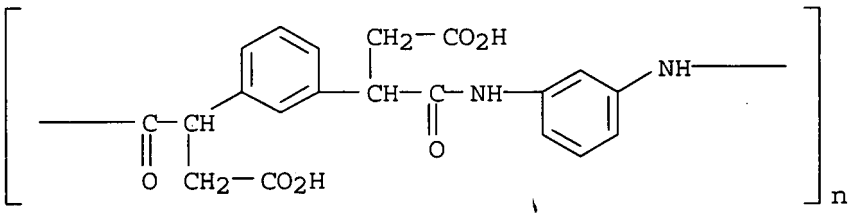
AB Monoesterification of HO2CCH2CHPhCO2H with ROH (R = Me, Et, Me2CH, Bu, Me2CHCH2, cyclohexyl, PhCH2) followed by esterification with tropine gave diesters I (R1 = CO2R). Amidation of I (R1 = CO2Me) with NH4OH, MeNH2 PhCH2NH2, and PhNH2 gave I (R1 = CONHR2; R2 = H, Me, CH2Ph, Ph). I and their methiodide salts were tested for anticholinergic activity. I (R1 = CO2CH2CHMe2) showed antispasmodic activity comparable to that of atropine.
IT 114649-01-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antispasmodic activity of)
RN 114649-01-3 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(4-amino-1,4-dioxo-3-phenylbutoxy)-8,8-dimethyl-, iodide (9CI) (CA INDEX NAME)



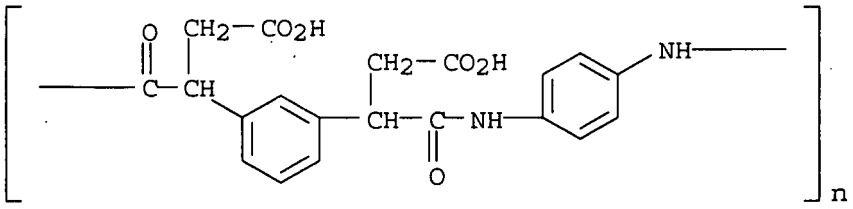
IT 114648-98-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, quaternization, and anticholinergic activity of)
RN 114648-98-5 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester (9CI) (CA INDEX NAME)



L17 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1987:102756 CAPLUS
DN 106:102756
TI Aliphatic polyimides from phenylene bis(succinic anhydride) and bis(glutaric anhydride)
AU Teshirogi, Takuma
CS Macromol. Res. Lab., Yamagata Univ., Yonezawa, 992, Japan
SO Journal of Polymer Science, Part A: Polymer Chemistry (1987), 25(1), 31-6
CODEN: JPACEC; ISSN: 0887-624X
DT Journal
LA English
AB m- And p-derivs. of phenylene bis(succinic anhydride) and bis(glutaric anhydride) were obtained from 1,3- [77104-43-9] and 1,4-bis(β-cyano-β-carbethoxyvinyl)benzene [47375-13-3] with KCN or Meldrum's acid followed by hydrolysis with concentrated HCl and dehydration with Ac2O. Aliphatic polyimides were prepared from these anhydrides with 6 aromatic diamines through thermal ring closure of polyamic acids obtained by solution polymerization in AcNMe2, and thermal stability of these polyimides was examined by thermogravimetric anal.
IT 107039-92-9P 107039-93-0P 107039-94-1P
107040-11-9P 107040-12-0P 107065-64-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and reduced viscosity of)
RN 107039-92-9 CAPLUS
CN Poly[imino-1,3-phenyleneimino[2-(carboxymethyl)-1-oxo-1,2-ethanediyl]-1,3-phenylene[1-(carboxymethyl)-2-oxo-1,2-ethanediyl]] (9CI) (CA INDEX NAME)

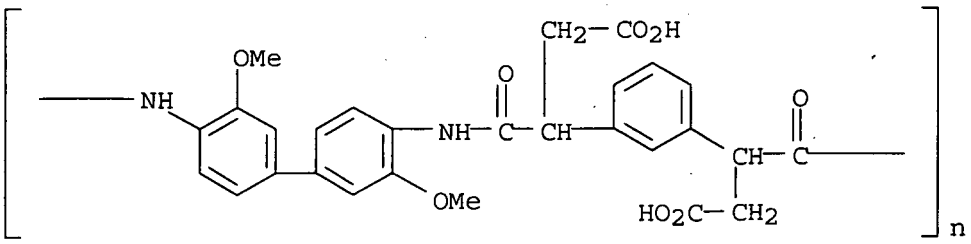


RN 107039-93-0 CAPLUS
CN Poly[imino-1,4-phenyleneimino[2-(carboxymethyl)-1-oxo-1,2-ethanediyl]-1,3-phenylene[1-(carboxymethyl)-2-oxo-1,2-ethanediyl]] (9CI) (CA INDEX NAME)

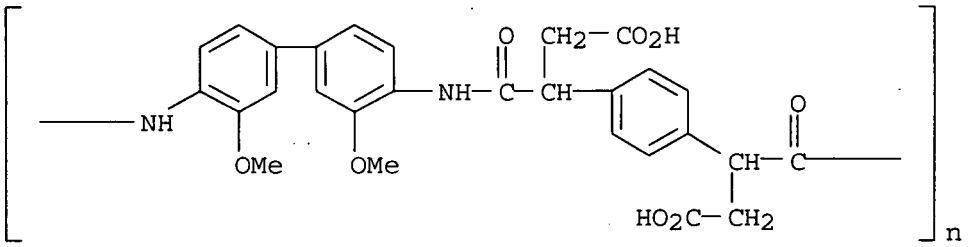


RN 107039-94-1 CAPLUS
CN Poly[imino(3,3'-dimethoxy[1,1'-biphenyl]-4,4'-diyl)imino[2-(carboxymethyl)-

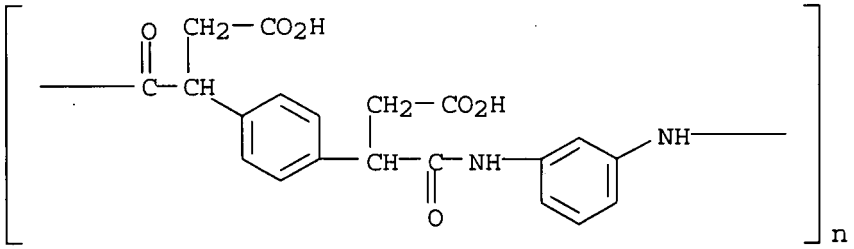
1-oxo-1,2-ethanediyl]-1,3-phenylene[1-(carboxymethyl)-2-oxo-1,2-ethanediyl]] (9CI) (CA INDEX NAME)



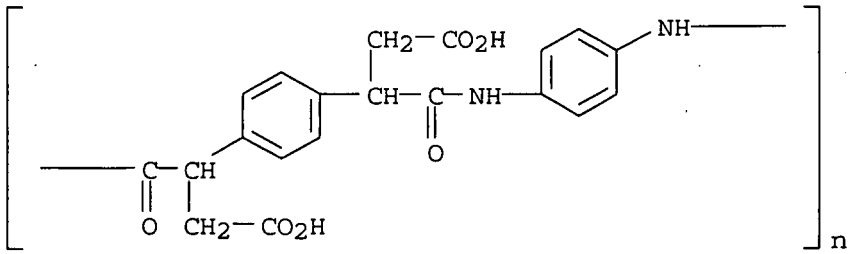
RN 107040-11-9 CAPLUS
CN Poly[imino(3,3'-dimethoxy[1,1'-biphenyl]-4,4'-diyl)imino[2-(carboxymethyl)-1-oxo-1,2-ethanediyl]-1,4-phenylene[1-(carboxymethyl)-2-oxo-1,2-ethanediyl]] (9CI) (CA INDEX NAME)



RN 107040-12-0 CAPLUS
CN Poly[imino-1,3-phenyleneimino[2-(carboxymethyl)-1-oxo-1,2-ethanediyl]-1,4-phenylene[1-(carboxymethyl)-2-oxo-1,2-ethanediyl]] (9CI) (CA INDEX NAME)



RN 107065-64-5 CAPLUS
CN Poly[imino-1,4-phenyleneimino[2-(carboxymethyl)-1-oxo-1,2-ethanediyl]-1,4-phenylene[1-(carboxymethyl)-2-oxo-1,2-ethanediyl]] (9CI) (CA INDEX NAME)

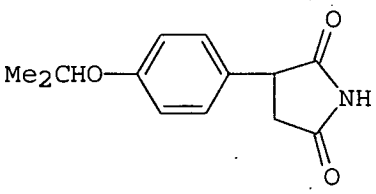


CAS ONLINE PRINTOUT

L17 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1979:611103 CAPLUS
DN 91:211103
TI Antispasmodic
IN Mndzhoyan, O. L.; Avetisyan, S. A.; Akopyan, N. E.; Gerasimyan, D. A.
PA Institute of Fine Organic Chemistry, Academy of Sciences, Armenian S.S.R., USSR
SO Ger. Offen., 26 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 2759051	A1	19790712	DE 1977-2759051	19771230
PRAI DE 1977-2759051	A	19771230		

GI

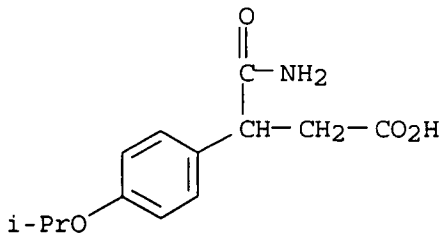


I

AB The phenylsuccinimide I, useful as a muscle relaxant in treating epilepsy with mild seizures, was prepared Thus, 4-Me2CHOC6H4CH(CO2H)CH2CO2H was warmed 2-3 h with Ac2O to give the corresponding succinic anhydride, which, in EtOAc, was treated with NH3-Et2O to give the 2 isomeric α-(4-isopropoxyphenyl)succinamidic acids. These were cyclized by heating to 200-20° with H2O removal to give 68-70% I. Tests of I with mice and rats gave ED50 86, 110, 77, and 90 mg/kg as a muscle relaxant in the korasol, strychnine, electroshock, and camphor tests, resp.

IT 72058-22-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

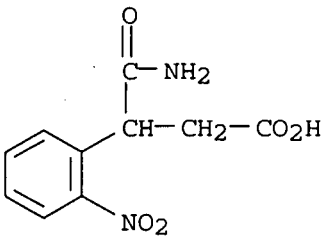
RN 72058-22-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-(1-methylethoxy)- (9CI) (CA INDEX NAME)



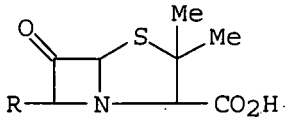
L17 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1977:534195 CAPLUS
DN 87:134195

CAS ONLINE PRINTOUT

TI Preparation of o-nitrophenylsuccinic acid and of some functional derivatives
AU Cuiban, F.; Lupea, Alfa; Silasi, Marcela; Sora, Mariana
CS Chem. Eng. Fac., Polytech. Inst. "Traian Vuia", Timisoara, Rom.
SO Revue Roumaine de Chimie (1977), 22(6), 869-75
CODEN: RRCHAX; ISSN: 0035-3930
DT Journal
LA English
OS CASREACT 87:134195
AB Nitration of HO2CCHPhCH2CO2H with HNO3 gave 17% o-nitrophenylsuccinic acid (o-I) and 83% p-I. The nitration of phenylsuccinic anhydride with AcONO2 gave 35% o-I and 65% p-I. O-I was also prepared from o-O2NC2H2CHO via o-O2NC6H4CH:C(CO2Et)2.
IT 63508-60-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 63508-60-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-2-nitro- (9CI) (CA INDEX NAME)



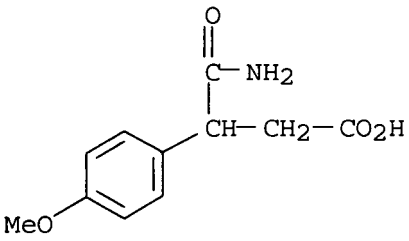
L17 ANSWER 11 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1977:439351 CAPLUS
DN 87:39351
TI Studies of semisynthetic penicillins. XI. The 6-aminopenicillane derivatives of p-alkoxyphenyl- and p-alkoxybenzylsuccinic acids. Ester penicillins
AU Mndzhoyan, Sh. L.; Manucharyan, I. Z.; Bil'bulyan, S. Z.; Ter-Zakharyan, Yu. Z.; Paronikyan, R. V.; Kazaryan, E. V.; Mndzhoyan, A. L.
CS Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
SO Khimiko-Farmatsevticheskii Zhurnal (1977), 11(3), 49-53
CODEN: KHFZAN; ISSN: 0023-1134
DT Journal
LA Russian
GI



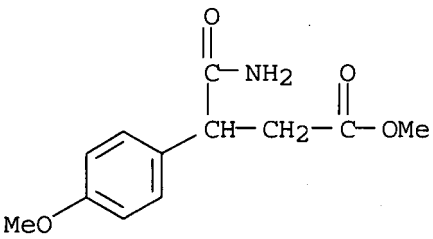
I, R=R1CH(CO2Me)CH2CONH
II, R=R1CH(CH2CO2Me)CONH

AB Penicillanic acid derivs. I and II [R1 = p-(C1-4 alkoxy)phenyl, p-(C1-4 alkoxy)benzyl] were obtained in 40-64% yields by treating 6-aminopenicillanic acid with the corresponding Me esters of succinic acid. I and II are effective bactericides.
IT 38499-25-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of)
RN 38499-25-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-methoxy- (9CI) (CA INDEX NAME)



IT 63151-92-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deamidation of)
RN 63151-92-8 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)



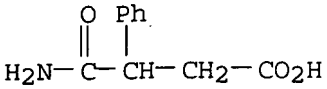
L17 ANSWER 12 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1977:67459 CAPLUS
DN 86:67459
TI Colorimetric hydroxylamine-iron(III) methods for studies of the enzymic hydrolyses of cyclic imides and of amic acids
AU Maguire, James H.; Dudley, Kenneth H.
CS Sch. Med., Univ. North Carolina, Chapel Hill, NC, USA
SO Analytical Chemistry (1977), 49(2), 292-7
CODEN: ANCHAM; ISSN: 0003-2700
DT Journal
LA English
AB An application of the hydroxylamine-Fe(III) method for the colormetric determination of amides as hydroxamic acids is described. The method was developed for studies of the enymic hydrolysis of a cyclic imide to its ring-opened product, an amic acid. The method, in which the derivatization reaction between an amic acid and hydroxylamine is performed at pH 7 and 94°, permits observation of the appearance of an amic acid in an incubation mixture of a cyclic imide with enzyme (e.g., dihydropyrimidinase, EC 3.5.2.2). The method also permits observation of the disappearance of an amic acid in an incubation mixture of an amic acid with enzyme (e.g., ω-amidase, EC 3.5.1.3). Assays were developed for studies of the enzymic hydrolysis of the following compds.: succinimide and succinamic acid, α-phenylsuccinimide and 2- and 3-phenylsuccinamic acid, glutarimide and glutaramic acid,

α-phenylglutarimide and 2- and 4-phenylglutaramic acid, and adipimide and adipamic acid.

IT 712-56-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, enzymic, hydroxylamine-iron methods in study of)

RN 712-56-1 CAPLUS

CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1972:539560 CAPLUS

DN 77:139560

TI Ammonolysis of p-alkoxyphenylsuccinic acid anhydrides

AU Avetisyan, S. A.; Midzhoyan, O. L.

CS Inst. Tonkoi Org. Khim. im. Mndzhoyana, Erevan, USSR

SO Armyanskii Khimicheskii Zhurnal (1972), 25(6), 512-17
CODEN: AYKZAN; ISSN: 0515-9628

DT Journal

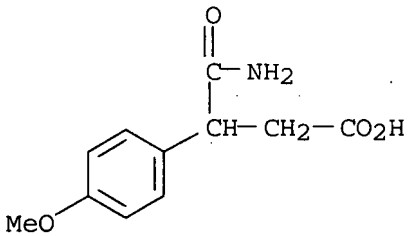
LA Russian

AB Ammonolysis of p-alkoxy-phenylsuccinic acid anhydrides gave an α-isomer, p-ROC6H4CH-(CONH2)CH2CO2H (R = Me, Et, Br), and larger amts. of a β-isomer, p-ROC6H4CH(CO2H)CH2CONH2, compared with the unsubstituted phenyl analogs which gave the opposite ratio of α- and β-isomers. The increase in the β-isomer with alkoxy substitution was explained by its resonance effect.

IT 38499-25-1P 38499-26-2P 38499-27-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 38499-25-1 CAPLUS

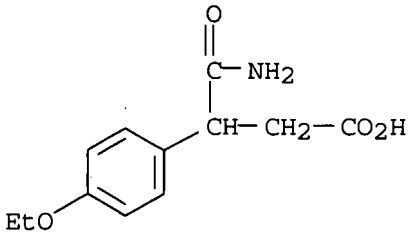
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-methoxy- (9CI) (CA INDEX NAME)



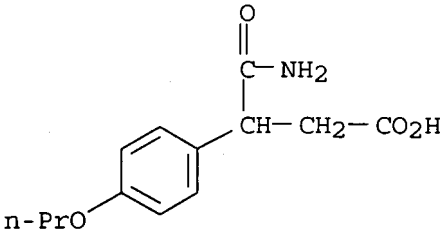
RN 38499-26-2 CAPLUS

CN Benzenepropanoic acid, β-(aminocarbonyl)-4-ethoxy- (9CI) (CA INDEX NAME)

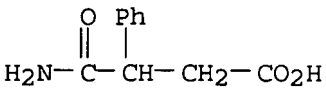
CAS ONLINE PRINTOUT



RN 38499-27-3 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-propoxy- (9CI) (CA INDEX NAME)

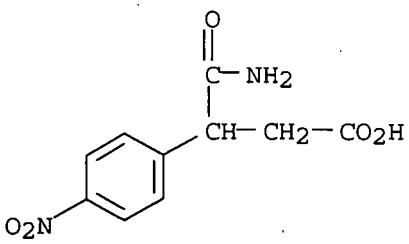


L17 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1972:107806 CAPLUS
DN 76:107806
TI Metabolic fates of N-methyl-α-phenylsuccinimide (phensuximide, Milontin) and of α-phenylsuccinimide in the dog
AU Dudley, Kenneth H.; Bius, Daniel L.; Grace, Michael E.
CS Sch. Med., Univ. North Carolina, Chapel Hill, NC, USA
SO Journal of Pharmacology and Experimental Therapeutics (1972), 180(1), 167-79
CODEN: JPETAB; ISSN: 0022-3565
DT Journal
LA English
AB 2-Phenylsuccinamic acid (I) [34367-66-3] isolated from urine of dogs receiving either RS-phensuximide (II) [34367-67-4] or RS-α-phenylsuccinimide (III) [34367-68-5] was essentially the optically pure levo-form which had the R-configuration. No α-(p-hydroxyphenyl)succinimide [32856-94-3] nor 3-phenylsuccinic acid [34367-69-6] was found as a metabolite of II or III. The same absolute configuration of R(-)-I and of R(-)-phenylhydantoic acid [6489-76-5] suggested that the same enzyme may be responsible for these stereospecific reactions of opening of the succinimide and hydantoin rings.
IT 712-56-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 712-56-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



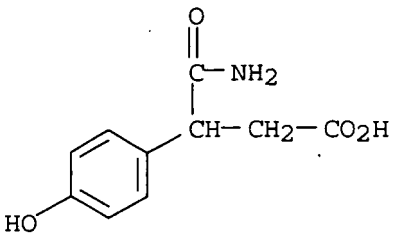
CAS ONLINE PRINTOUT

L17 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1971:448634 CAPLUS
DN 75:48634
TI Derivatives of dibasic carboxylic acids. XXXV. Addition to hydrogen cyanide to the double bond of p-substituted benzylidene malonates, and the preparation of succinimides
AU Avetisyan, S. A.; Mndzhoyan, O. L.
CS Inst. Tonkoi Org. Khim., Erevan, USSR
SO Armyanskii Khimicheskii Zhurnal (1971), 24(3), 252-8
CODEN: AYKZAN; ISSN: 0515-9628
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Title compds. were prepared as potential anticonvulsive agents. A mixture of 0.2 mole of p-ROC6H4CH:C(CO2Et)2 in 500 ml EtOH and 0.202 mole KCN in 50 ml H2O heated 18 hr at 65° gave p-ROC6H4CH(CN)CH2CO2Et (I) (R = alkyl). p-O2NC6H4CH:C(CO2Et)2 and KCN in aqueous EtOH heated 18 hr at 65° gave p-O2NC6H4CH(CONH2)CH2CO2H, (II) and p-O2NC6H4CH(CN)CH2CO2H, and with HCl, p-O2NC6H4CH(CO2H)CH2CO2H (III). I kept with NaOMe in MeOH 24 hr at room temperature gave p-ROC6H4CH(CN)CH2CO2H. III reduced with Sn and HCl gave p-H2NC6H4CH(CO2H)CH2CO2H (IV). III, N2H4.H2O, EtOH, and Raney Ni heated 6 hr at 65° and filtered gave III.N2H4 and IV. A mixture 6N NH4OH and III saturated with H2S at 5° gave IV. III, MeOH, C6H6, and H2SO4 refluxed 5 hr gave p-O2NC6H4CH(CO2Me)CH2CO2Me (V). V reduced with Ni and N2H4 as above gave p-H2NC6H4CH(CO2H)CH2CO2H.N2H4, and p-H2NC6H4CH(CO2Me)CH2CO2Me. p-HOC6H4CH(CO2H)CH2CO2H treated with Ac2O gave the cyclic anhydride, which treated with NH4OH gave p-HOC6H4CH(CONH2)CH2CO2H. This heated 30 min at 200° gave VI (R = OH). III and Ac2O refluxed 6 hr and worked up via NH3 in ether gave II.NH3, which gave II. II and Ac2O heated 6 hr at 100° gave VI (R = NO2). IV and Ac2O heated 2 hr at 100° gave a solid, m. 155°, which dissolved in ether, treated with NH3, evaporated and heated 1 hr at 200° gave a solid, which treated with etheral HCl gave VI.HCl (R = NH2) (VII.HCl), which in acetone treated with ethereal NH3 gave VII.
IT 32856-83-0P 32856-93-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 32856-83-0 CAPLUS
CN Succinamic acid, 3-(p-nitrophenyl)- (7CI, 8CI) (CA INDEX NAME)

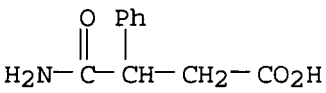


RN 32856-93-2 CAPLUS
CN Succinamic acid, 3-(p-hydroxyphenyl)- (8CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT



L17 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1965:2846 CAPLUS
DN 62:2846
OREF 62:474a-b
TI The action of ammonia on? α,α-disubstituted succinoyl chlorides. Preparation of succinoyl acid nitriles
AU Foucaud, Andre; Plusquellec, Paul
CS Fac. Sci. Rennes, Fr.
SO Compt. Rend. (1964), 259(11), 1875-7
DT Journal
LA French
AB cf. CA 59, 5069d. Reaction of phenylsuccinoyl chloride with NH3 according to Wideqvist (CA 49, 6121a) and acid hydrolysis of the nitrile formed gave a mixture, which was separated by chromatography or recrystn. from 80% EtOH into
75% PhCH(CO2H)CH2CONH2, m. 168-9°, and 25% PhCH(CONH2)CH2CO2H, m. 171°. Treatment of α,α-benzylphenylsuccinoyl chloride with NH3 gave 90% PhCH2CPh(CO2H)CH2CN.0.5H2O, m. 175°, ν 1708 (CO), 2241 cm.-1 (CN) (Nujol). The isomeric PhCH2CPh(CN)CH2CO2H showed ν 1727 and 2259 cm.-1 α,α-Diphenylsuccinoyl chloride and NH3 gave 40% Ph2C(CO2H)CH2CN, m. 176-8°, ν 1718, 1168 cm.-1 (Nujol), (the isomeric compound has ν 1699, 2237 cm.-1), and 40% Ph2C:C(CN)CONH2, m. 240° (95% EtOH). The reaction mechanism is discussed.
IT 712-56-1P, Succinamic acid, 3-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 712-56-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



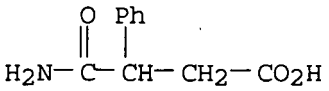
L17 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1963:428315 CAPLUS
DN 59:28315
OREF 59:5069d-h,5070a-c
TI Cleavage of α- and α,α-disubstituted succinic anhydrides. Action of ammonia and amines
AU Foucaud, Andre
CS Univ. Rennes
SO Bulletin de la Societe Chimique de France (1963), (4), 873-6
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB PhCH2Ac and NCCH2CO2Me condensed according to Cope, et al. (CA 36, 10118)

gave 70% PhCH2CMe:C(CN)CO2Me (I), b4 148-53°, n20D 1.5460. I (15 g.) in 20 ml. MeOH treated with 5 g. KCN in 20 ml. H2O, the mixture acidified with dilute HCl and extracted with Et2O, and the dried (Na2SO4) extract distilled yielded 70% colorless, oily PhCH2CMe(CN)CH(CN)CO2Me, b2 166-70°, n20D 1.5190, refluxed (5 g.) 4 hrs. in 100 ml. 2N aqueous Na2CO3 and the cooled solution extracted with Et2O to yield 90% Ph2CH2CMe(CN)CH2CN (II), b2 163-5°. II (5 g.) refluxed 3 hrs. in 120 ml. 0.5N NaOH in EtOH-H2O, the cooled solution acidified with dilute HCl and the precipitate taken up in Et2O and filtered gave 44% Et2O-insol. PhCH2CMe(CO2H)CH2CONH2 (III), m. 183-4° (80% alc.). The Et2O solution extracted with aqueous N NaHCO3 and the extract acidified gave 20% of the corresponding diacid, PhCH2CMe(CO2H)CH2CO2H (IV), m. 144° (alc.). The residual Et2O evaporated and the residue crystallized from alc. yielded 10% imide (V), m. 77-8°. IV (3 g.) refluxed 1 hr. in 20 ml. SOCl2, excess SOCl2 evaporated, the residue distilled, and the oil (2.2 g., b2 138-40°) refrigerated yielded 72% anhydride (VI) (R = PhCH2, R' = Me) (VII), m. 58-9° (CCl4). III (5 g.) neutralized with 2N Na2CO3 and shaken 5 hrs. at 0° with Me2SO4 yielded 50% PhCH2CMe(CO2Me)CH2CONH2 (VIII), m. 110-12°. The Na2CO3 solution acidified gave unreacted III and a small amount of V. VIII (2.6 g.) in 16 g. H2SO4 at 0° stirred at 0° with addition of 6 ml. aqueous 4M NaNO2 and the mixture stirred 30 min., poured onto ice, and extracted with Et2O gave PhCH2CMe(CO2Me)CH2CO2H, taken up (1.5 g.) at 0° in 7 ml. fuming H NO3 and poured onto ice, filtered and crystallized from 50% AcOH to give p-O2NC6H4CH2CMe(CO2Me)CH2CO2H, m. 103°. VI (R = R' = Me) (IX) was obtained by the action of AcCl on the corresponding diacid and the acid RR'C(CN)CH2CO2H (X) (R = R' = Me) (XI) by the procedure of Wideqvist (CA 45, 10217e). XI kept 4 days in H2O at 0° and the product washed with Et2O to remove unchanged XI yielded 30% RR'C(CONH2)CH2CO2H (XII) (R = R' = Me) (XIII), m. 134-5°. VI (RPhCH2, R' = H) (XIV) and X (R = PhCH2, R' = H) (XV) were obtained by standard procedures. XV (1 g.) in 5 ml. 85% H2SO4 at 0° poured onto 20 g. ice and the precipitate crystallized from 80% alc. gave XII(R = PhCH2, R' = H)(XVI). VI(R = R' = Ph; R = Ph, R' = H; R = Ph, R' = Et) (XVI, XVII, XVIII) were prepared according to the literature. VI (600 mg.) in dry Et2O at 20° saturated with dry NH3 or treated with H2NR in Et2O, the Et2O evaporated and the residue treated with dilute HCl, filtered and the precipitate dried gave 98-9% crude mixture of acid amides. Hyflosupercel (50 g.) kept 24 hrs. in 300 ml. 15% HCl, filtered, washed thoroughly with H2O and Me2CO, and the acid-free product dried 24 hrs. at 100°, mixed with K phosphate buffer (2M at a determined pH), and dried gave a powder containing 33% fixed phase. The powder was transformed to a paste with the mobile phase (CHCl3-BuOH saturated with buffer) and added to a column (30 ± 1 cm.) and washed with 50 ml. mobile phase. The acid amide mixture (7-13 mg.) in 2-3 ml. mobile phase chromatographed and eluted, IV bubbled through the fractions (4-5 ml.) and the frac-ions titrated with 0.01N NaOMe (cresol red) gave values from which an elution curve was traced. The chromatographic separation gave the 2 isomeric acid amides. Action of NH3 on VI gave a mixture of RR'C(CO2H)CH2CONH2 (XIX) and XII [anhydride, % XIX (pK), and % XII (pK) given]: XVII, 46.5 (4.71), 53.5-(4.95); XVI, 53(4.65), 47(5.21); XIV, 55.5(-), 44.5(4.80); VI (R = p-NO2C6H4, R' = H), 60(4.23), 40(4.53); VI (R = p-O2NC6H4, R' = Et), 67(4.28), 33(4.52); XVIII, 70(4.79), 30-(4.91); VI (R = p-O2NC6H4, R' = Me), 69.5(4.36), 30.5(4.66); VI (R = PhCH2, R' = Ph), 72(4.95), 28(5.14); IX, 76(5.25), 24-(5.20); VI (R = Ph, R' = Me), 78(4.89), 22(4.97); VII, 96-(5.21), -(-). With the exception of XVII, the XlX predominated. The following RR1C(CO2H)CH2CONR2R3 were isolated: R = R1 = Me, R2 = R3 = H, m. 125°; R = Et, R1 = Ph, R2 = R3 = Me, m. 163-4°; R = Ph, R1 = H, R2 = R3 = Me, m. 160-2°. The mechanism of the ring opening of the anhydrides was discussed.

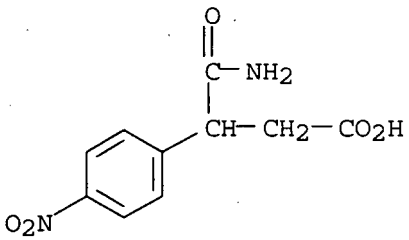
IT 712-56-1P, Succinamic acid, 3-phenyl- 32856-83-0P,

CAS ONLINE PRINTOUT

Succinamic acid, 3-(p-nitrophenyl)-
RL: PREP (Preparation)
(preparation of)
RN 712-56-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



RN 32856-83-0 CAPLUS
CN Succinamic acid, 3-(p-nitrophenyl)- (7CI, 8CI) (CA INDEX NAME)



L17 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1961:17767 CAPLUS
DN 55:17767
OREF 55:3516e-i,3517a-g
TI Synthesis and study of the cleavage of asymmetrically disubstituted succinic anhydrides and imides
AU Foucaud, Andre
CS Univ. Rennes, Fr.
SO Bulletin de la Societe Scientifique de Bretagne (1960), 35, 88 pp.
CODEN: BSSBAS; ISSN: 0037-9581
DT Journal
LA Unavailable
AB cf. Le Moal, CA 50, 14547b. Certain α-phenyl-α-(R-substituted)succinic anhydrides (I) and imides (II) were prepared, hydrolyzed, and the ratio of the resulting isomeric amide-acids was determined by partition chromatography. Condensation of PhCOR and NCCH2CO2R' gave PhCR:C(CN)CO2R' (III) (R, R', m.p. or b.p./mm. of one isomer given): PhCH2, Et (IIIa) 66°; PhCH2, Me, 195-200°/3; Et, Et, 46-7°; Et, Me, 151-2°/5 (m. 16°); Me, Me, 137-8°/2 (m. 70°). IIIa was hydrolyzed in 20% NaOH to give PhCH2CPh:CHCONH2, m. 186°. IIIa heated at 250° gave 2-cyano-3-phenyl-1-naphthol, m. 183° (xylene). III was refluxed with dilute alc. KCN solution and acidified to give NCCRPhCH(CN)CO2R' (IV) (R, R', m.p. or b.p./mm., % yield given): PhCH2, Et, 86°, 60; PhCH2, Me, 114°, -; Et, Et, 175-8°/1 (m. 52°), 67; Et, Me, 190-2°/3 (m. 62°), 60; Me, Me, 65°, 100. IV (R = Et) was hydrolyzed in cold concentrated H2SO4 to give quant. H2NCOCPhRCH(CONH2)CO2Et (V) (R = PhCH2) (Va), m. 175-6°; V (R = Et) m. 165°. Alkaline hydrolysis of V gave 3-phenyl-3-(R-substituted)-4-carbamoylsuccinimide (R = PhCH2) (VI), m. 198-200°; VI (R = Et) (VIa) m. 180°. VI was also obtained by fusion of Va. IV refluxed 0.5 hr. in dilute alc. N Na2CO3 yielded quant. NCC-PhRCH2CN (VII) (R and m.p. or b.p./mm. given): PhCH2 (VIIa), 103°; Et (VIIb), 165-70°/3 (m. 38°);

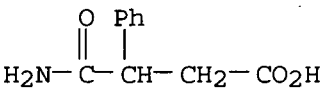
Me, 29°. When the above basic solution of IV was acidified it yielded 3-phenyl-3-(R-substituted)-4-cyanosuccinimides with R = PhCH2, m. 169°, and R = Et (VIII), m. 117°. VIII hydrolyzed in concentrated H2SO4 gave VIa. VII was hydrolyzed in aqueous alc. KOH, acidified, and the precipitate extracted with Et2O to obtain quant. from dilute AcOH HO2CCPhRCH2CO2H (IX)
(R and m.p. given): PhCH2, 220°; Et, 156°; Me, 167°.
VIIa (5 g.) refluxed 8 hrs. with 20.4 g. concentrated H2SO4, 12.9 g. AcOH, and 4.1 g. H2O gave 80% 3-carboxy-3-phenyl-1-tetralone, m. 192°; 2,4-dinitrophenylhydrazone m. 280°. VIIa in cold concentrated H2SO4 24 hrs. gave 80% H2NCOC(CH2Ph)PhCH2CONH2 (X), m. 200°, which hydrolyzed quant. in dilute NaOH to II (R = PhCH2). VII refluxed in dilute alc. 0.25N NaOH 0.5 hr. yielded 70% NCCPhRCH2CONH2 (XI) (R = PhCH2) (XIa), m. 245-7°; XI (R = Et) m. 228°. XIa formed an HCl salt, m. 170° (decomposition). XIa was also prepared by heating NCC(CH2Ph)PhCH2CO2NH4 to 250°. VIIb heated 1 hr. with dilute alc. N NaOH and acidified gave 70% II (R = Et), m. 99°. II (R = Me), m. 88°, was similarly prepared The IX and II were treated with ice-cold concentrated HNO3 15 min. to give 4-O2NC6H4CR(CO2H)CH2CO2H (XII) and 4-O2NC6H4CR.CO.NH.CO.CH2 (XIII), resp. (compound, R, m.p., and % yield given): XII, Et, 218-20°, 60; XII, Me, 168°, 56; XIII, Et, 132-3°, 75; XIII, Me, 156°, 60. By heating IX and XII with SOCl2, I and 4-O2NC6H4CR.CO.O.CO.CH2 (XIV), resp., were obtained (compound, R, and m.p. or b.p./mm. given): I, PhCH2, 112°; I, Et, 165-70°/6; I, Me, 140°/2; XIV, Et, 104-5°; XIV, Me, 123-4°; XIV, H, unrectifiable oil. To prepare asym. disubstituted succinamic acids of known structure, 18 g. PhCH2CHPhCN was treated with a solution of tert-BuONa (XV) (from 2.3 g. Na and 16 g. tert-BuOH in 300 ml. benzene) and 17 g. BrCH2CO2Et to give NCCPhRCH2CO2R' (XVI) (R = PhCH2, R' = Et), m. 62°, which was saponified to XVI (R = PhCH2, R' = H) (XVIa), m. 163°, in 51% over-all yield. XVI (R = R' = Et), b1 145-50°, was prepared analogously in 74% yield but with NaNH2 in lieu of XV, and saponification in cold alkaline 93 % MeOH solution led to XVI (R = Et, R' = H), m. 75°, via the Na salt. XVI (R = Me, R' = H), m. 84°, was similarly prepared XVI (R = Ph or H, R' = H) were hydrolyzed in cold concentrated H2SO4 to H2NCOCPhRCH2CO2H (XVII) (R = Ph), m. 159°, and XVII (R = H), m. 172°. XVI (R = Et or Me, R' = H) were hydrolyzed in dilute neutral alc. to XVII (R = Et), m. 198°, and XVII (R = Me), m. 172°. HO2CCPhRCH2CONH2 (XVIII) (R = H), m. 162°, was obtained from the corresponding nitrile in H2SO4. XVIa did not hydrolyze to the amide-acid but in H2SO4 formed I (R = PhCH2). XVIa with SOCl2 then NH4OH gave a compound, C17H16N2O, m. 143°, presumably 2,5-diimino-3-phenyl-3-benzyltetrahydrofuran, which formed XIa in cold alc. N NaOH. XVII and XVIII gave on nitration 4-O2NC6H4C(CONH2)RCH2CO2H (XVIIIa) (R = H), m. 188°, XVIIIa (R = Et), m. 184-6°, XVIIIa (R = Me), m. 189-90°, and 4-O2NC6H4C(CO2H)RCH2CONH2 (XIX)(R = H), m. 200°, resp. The I were converted to mixts. of isomeric amide-acids by passage of NH3 through an Et2O solution followed by acidification of an aqueous solution of the resulting salts, extraction with Me2CO, and evaporation Partition chromatography on kieselguhr at 20° with BuOH-CHCl3 as the mobile phase afforded separation of the isomers (anhydride, R, % α-substituted-β-amide formed, and pH of stationary phase given): I, H, 46.6, 6.40; XIV, H, 60.3, 6.17; I, Ph, 53.2, 7.35; I, PhCH2, 72.2, 6.20; I, Et, 70.2, 7.35; I, Me, 78, 6.17; XIV, Et, 67, 6.39; XIV, Me, 69.6, 6.00. Similar results were obtained by hydrolysis of the II in hot alkaline solution From the chromatographic eluates the following succinamic acids were isolated and characterized (compound, R, and m.p. given): XVIII, Ph, 146°; XVII, PhCH2, 202-5°; XVIII, PhCH2, 230-2°;

XVIII, Et, 140°; XVIII, Me, 153-5°; XIX, Et, 170° (decomposition); XIX, Me, 180-2°. The pK of the succinic α-ester-β-acids was higher than that of the isomeric β-ester-α-acids when either was substituted at α by (a) one or (b) two Ph or (c) by Ph and PhCH2. The amide-acids behaved similarly in cases (a) and (b) and presumably also in (c). An interpretation of the results on the basis of inductive and steric effects of the substituents was presented. 41 references.

IT 712-56-1P, Succinamic acid, 3-phenyl- 32856-83-0P, Succinamic acid, 3-(p-nitrophenyl)-
RL: PREP (Preparation)
(preparation of)

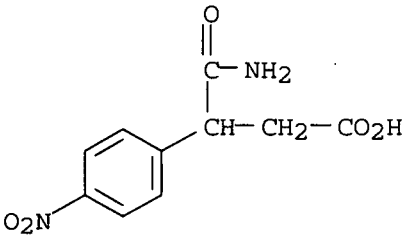
RN 712-56-1 CAPLUS

CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



RN 32856-83-0 CAPLUS

CN Succinamic acid, 3-(p-nitrophenyl)- (7CI, 8CI) (CA INDEX NAME)



L17 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1952:5424 CAPLUS

DN 46:5424

OREF 46:936i,937a

TI Hydrolysis of β-phenyl-β-cyanopropionic acid

AU Wideqvist, Sigvard

CS Univ. Uppsala, Swed.

SO Arkiv foer Kemi (1951), 3, 147-52
CODEN: ARKEAD; ISSN: 0365-6128

DT Journal

LA English

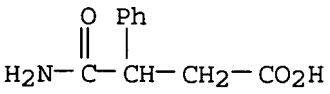
AB cf. C.A. 39, 2023.4. PhCH(CN)CH2CO2H, prepared by the method of W. (C.A. 37, 5046.4), hydrolyzes spontaneously in aqueous solution at room temperature to PhCH(CONH2)CH2CO2H. A formula is derived for the calcn. of the hydrolysis velocity constant from conductivity data with the assumption that the hydrolysis is partly catalyzed and partly uncatalyzed by H ion, and that the undissocd. cyano acid hydrolyzes. The velocity consts. for the uncatalyzed (k1 = 1.10 + 10-4) and the catalyzed (k2 = 1.13 + 10-2) reactions were determined by conductivity measurements at 25°.

IT 712-56-1P, Succinamic acid, 3-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 712-56-1 CAPLUS

CAS ONLINE PRINTOUT

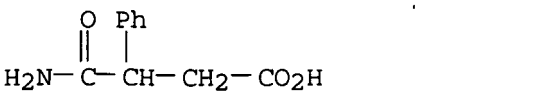
CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



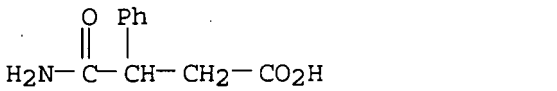
L17 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1943:31434 CAPLUS
DN 37:31434
OREF 37:5046d-i
TI Phenylcyano-substituted carboxylic acids
AU Wideqvist, Sigvard
SO Svensk Kem. Tid. (1942), 54, 34-8
From: Chem. Zentr. II, 889-90(1942).
DT Journal
LA Unavailable
AB A new general method is described for the preparation of substituted carboxylic acids in which a Ph and a CN group are attached to the same C atom. The starting material is Ph(NC)CHCO2Et (I), prepared from PhCH2CN and Et2CO3 with Na (Hessler, Am. Chemical J. 32, 127(1904). The Na salt (II) of I can be condensed with haloaliph. esters (e. g., ClCH2CO2Et) to give succinic esters which with alc. alkali are decarboxylated to 53-89% of the Ph(NC)CH(CH2)xCO2H. Those acids which contain the CN group in the β-position are easily hydrolyzed to the corresponding amides. Warming II and ClCH2CO2Et in EtOH on the water bath, dilution with H2O and extraction with ether-C6H6 give 81% of di-Et α-phenyl-α-cyanosuccinate, b8 190-3°; hydrolysis with alc. KOH on the water bath and acidification give 89% of β-phenyl-β-cyanopropionic acid (III), m. 75°; the dissociation constant (k25) is 1.62 + 10-4 (graphically extrapolated). The action of H2O upon III at room temperature gives the amide, PhCH(CONH2)CH2CO2H, m. 158-9°, k25 3.76 + 10-5. Reduction of an aqueous suspension of PhCH:C(CN)CO2Et with Na-Hg in a CO2 atmospheric gives 86% of β-phenyl-α-cyanopropionic acid, m. 101°, k25 5.70 + 10-3. II and MeCHBrCO2Et give 60% of di-Et α-methyl-β-phenyl-β-cyanosuccinate, b8 185-9°; hydrolysis gives 85% of a mixture of the 2 diastereomeric α-methyl-β-phenyl-β-cyanopropionic acids (IV); hydrolysis of the mixture with concentrated H2SO4 and addition of NaNO2 gives a mixture, fractional crystallization from H2O yielding α-methyl-β-phenylsuccinic acid (V), m. 172-3° and 192-3° (cf. Zelinsky and Buchstab, Ber. 24, 1879(1891)). In NH4OH IV yields a difficultly soluble Ca salt which crystallizes from dilute MeOH in fine needles and gives a IV m. 99-100°, k25 2.0 + 10-4, which is hydrolyzed to a V m. 191°; the more easily soluble Ca salt of IV yields a IV m. 77-80°. II and Me2CBrCO2Et give 53% of di-Et α,α-dimethyl-β-phenyl-β-cyanosuccinate, b9 187-92°; this gives 75% of α,α-dimethyl-β-phenyl-β-cyanopropionic acid (VI), m. 116-17°, k25 1.12 + 10-4. Concentrated HCl and VI at 115° give α,α-dimethyl-β-phenylsuccinic acid (VII), m. 165°. Concentrated H2SO4 at room temperature converts VI into the monoamide of VII, m. 163-4°, k25 about 1.6 + 10-5. II and ClCH2CH2CO2Et give 82% of Et α-phenyl-α-cyanoglutarate, b8 197-8°; alc. KOH gives 75% of γ-phenyl-γ-cyanobutyric acid, m. 61°, k25 3.94 + 10-5; hydrolysis with concd, H2SO4 gives α-phenylglutaric acid monoamide, m. 168°, k25 2.31 + 10-5.
IT 712-56-1P, Succinamic acid, β-phenyl-

CAS ONLINE PRINTOUT

RL: PREP (Preparation)
(preparation of)
RN 712-56-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1941:25260 CAPLUS
DN 35:25260
OREF 35:3993g-i
TI β-Phenyl-β-cyanopropionic acid
AU Wideqvist, Sigvard
SO Arkiv. Kemi, Mineral. Geol. (1940), 14B(No. 19), 6 pp.
DT Journal
LA German
AB PhCH(CN)CH2CO2H (I) has been prepared according to Bredt and Kallen (Ann. 293, 338(1896)) and Anschutz (C. A. 1, 2702) by treating PhCH:C(CO2Et)2 (II) with 2 mols. KCN. The m. p. found for I differs from that reported by the previous investigators. To 62 g. II in 375 ml. alc. is added 33 g. KCN in 150 ml. H2O and the mixture is heated for 7 hrs. on the water bath. KHCO3 is filtered off and I, liberated by concentrated HCl, is obtained as an oil. I is purified through its Ca salt (III) which is crystallized from hot H2O in the presence of animal charcoal whereby 25 g. of pure III is obtained. III is decomposed with HCl, I extracted with ether, the ether evaporated, and the oily acid transformed into crystals by rubbing with a glass rod. I, crystals from C6H6, m. 75°. From dilute alc. I seps. as an oil. (B. and K. and A. obtained crystals from dilute alc., m. 150°.) By heating I with concentrated HCl for 3 hrs. in a sealed tube at 115° is obtained more than 90% PhCH(CO2H)CH2CO2H, m. 167°. By treating I with H2O at 25° for several days it is transformed into PhCH(CONH2)CH2CO2H, m. 157-8°.
IT 712-56-1P, Succinamic acid, β-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 712-56-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1914:4524 CAPLUS
DN 8:4524
OREF 8:703c-i,704a-h
TI Unsaturated compounds. X. Action of free hydroxylamine on coumarins
AU Posner, Theodor; Hess, Rudolf
CS Univ. Greifswald
SO Berichte der Deutschen Chemischen Gesellschaft (1914), 46, 3816-33
CODEN: BDCGAS; ISSN: 0365-9496
DT Journal

CAS ONLINE PRINTOUT

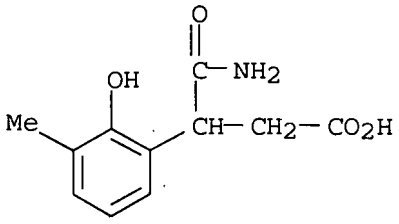
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A., 3, 2566; Francesconi and Cusmano, C. A., 4, 1741. Whether P.'s tri- (a) or F. and C.'s dihydroxylamino compound (b) is formed does not depend on the temperature, as believed by F. and C., but on the nature of the solvent and on whether there is present a slight excess of NaOH or of NH2OH.HCl. In the presence of alkaline in EtOH, only (b) is formed, even at o°, while in the absence of alkaline in EtOH or MeOH (a) is always formed at low temps. After 8 days in EtOH (a) passes into (b); in McOH, into the NH2 acid (c). P.'s former views as to the structure of (a) and (c) have been confirmed, and since (b) is formed as a secondary product from (a), it probably has the structure HOC6H4CH(NHOH)CH2C(:NOH)OH and not the cyclic structure given by F. and C. Of the 3 methylcoumarins with the Me in the o-, m- and p-positions to the O, none reacts with NH2OH nearly so easily and smoothly as with coumarin itself. 4-o-Hydroxyphenyldihydrouracil, from o-HOC6H4CH(NH2)CH2CO2H, KCNO and HCl, decomps. 239-41°, insol. in acids, NH2 and Na2CO3, soluble in NaOH. That in (c), m. 220°, the NH2 is in the β-position is shown by the fact that (c) depresses the m. p. (248°) of Blum's α-acid (Arch. exp. Path. Pharm., 59, 273) to 216°. (In the following, the notation is used.) 3-Methylcoumarin, obtained in 60% yield of the aldehyde by heating 27 g. 3,2-Me(HO)C6H3CHO with 20.8 g. CH2(CO2H)2 and 4 g. PhNH2.HCl at 100° and finally at 130-5° and decomposing the resulting acid (b18 240-5°) at 300°, b26 180-5°; with NH2OH in cold MeOH it yields a compound, probably β-hydroxyliminobis-o-hydroxy-m-methyl-β-phenylpropionhydroxamic acid, {Me(HO)C6H3CH[CH2C(:NOH)OH]}2NOH, decompose about 90-5°, easily soluble in NH3 and alks., less in H2O and dilute acids, does not reduce cold Fehling solution, gives a red-brown color with FeCl3. B. 8 hrs. with NH2OH in EtOH, the coumarin gives β-amino-β-2-hydroxy-3-methylphenylpropionic acid, powder, soluble in dilute acids, alks. and carbonates, begins to decompose 176° m. 184-5°; hydrochloride, decomps. 130-5°; silver salt, very unstable precipitate B. 1 hr. with 10 parts Ac2O, the acid gives the acetyl anhydride (2-acetylamino-3-methyldihydrocoumarin), powder, decompose 135-7°, insol. in NaOH, Na2CO3, and dilute acids. Benzoyl derivative of the acid, from 2 g. of the acid and 15 g. BzCl in excess of concentrate NaOH without cooling, crystalline powder, decompose 166-9°, soluble in alks. and soda, insol. in dilute acids. If 3 g. acid and 15 g. BzCl in 30 cc. cold H2O and 30 cc. dilute NaOH are used, the product is the benzoyl benzoate, crystalline powder, sinters 71-6°, decompose 100°. β-Ureino derivative, from 3 g. of the acid and 1.8 g. KCNO in 60 cc. H2O heated 1 hr. and evaporated on the H2O bath, dissolved in H2O and heated to b. with an equal volume of concentrate HCl, decompose 210-7°, soluble in alks., insol. in dilute acids. Ethyl ester of the NH2 acid, from the acid in absolute alc. treated 15 min. without cooling with HCl gas, seps. as the hydrochloride, decomps. 99-140°. 4-Methylcoumarin, obtained in 60% yield of the cresol from 40.3 g. m-MeC6H4OH and 50 g. malic acid gradually heated to 135° in 180 g. H2SO4, m. 126-7°, does not react with alc. NH2OH in the cold but when heated 5 hrs. it gives β-amino-β-2-hydroxy-4-methylphenylpropionic acid, m. 215-6° (decompose), soluble in dilute acids, alks. and NH3, does not reduce Fehling solution; hydrochloride, powder, decomps. 180-6°; benzoyl derivative, m. 186-7° (decompose), soluble in alks. and soda, insol. in dilute acids; benzoyl benzoate, m. 145-8° (decompose), soluble in alks. and soda, insol. in acids (both of the last 2 compds., when b. 5 hrs. with 10% alc. H2SO4, yield a benzoyl ethyl ester, softens 150°, m. 155-9° (decompose), soluble in alkaline); β-phenylureino derivative, from the acid and PhNCO in NaOH, m. 169-71° (decompose), soluble in alks. and carbonates, insol. in acids. In the prepare of the NH2 acid there is regularly obtained a by-product, probably 2-bz-methylbenzisoxazole-β-acetic acid (I), needles, m.

167-71° (decompose), soluble in alks., NH3 and soda, insol. in dilute acids, does not reduce hot Fehling solution, gives only a faint yellow-red color with FeCl3, is unchanged by dissolving in NaOH, adding NaNO3 and cautiously acidifying, whereas, if it were the isoxazolone (II) it should have formed a NO compound soluble in alks. with pink color. 5-Methylcoumarin with cold alc. NH3OH yields a hygroscopic yellow substance, decomps. 80-5°, cannot be purified, gives an oily precipitate with dilute acids, reduces cold Fehling solution, gives a brown-violet color with FeCl3; it is probably hydroxylamine 5-methyl-2-hydroxycinnamhydroxamate, Me(HO)C4H3CH:CHC(:NOH)OH.NH2OH. An addition product of NH2OH to the C:C bond was obtained, by short b., as a white tar which, on b. with alc., yielded β-amino-β-2-hydroxy-5-methylphenylpropionic acid (also obtained by b. the coumarin 10 hrs. with alc. NH2OH), needles, m. 198-202° (decompose), easily soluble in alks. and acids; hydrochloride, yellowish needles, decompose 157°; silver salt, precipitate exceedingly sensitive to light; diacetyl anhydride(?), obtained by b. the acid with Ac2O and pouring into cold H2O, m. 130-2°, cannot be recrystd.; benzoyl derivative, m. 170-5° (decompose), soluble in alks., insol. in dilute acids; benzoyl benzoate, softens 100°, m. 105-9° (decompose), soluble in alks. and soda, insol. in dilute acids; benzoyl ethyl ester, m. 120-1°, soluble in alks., insol. in acids; β-urcino derivative, m. 149° (decompose), soluble in alks., insol. in dilute acids, converted by heating to incipient b. with concentrate HCl into 4[-2-hydroxy-5-methylphenyl]dihydrourocil, begins to decompose 235°, m. 245°, soluble in alks., insol. in dilute acids; ethyl ester hydrochloride of the NH3 acid, decompose 149-50°. In the prepare of the NH2 acid is formed a by-product, darkens 149°, m. 155° (decompose), soluble in alks., insol. in dilute acids, gives a deep red color with FeCl3, does not reduce Fehling solution It is probably 3-bz-methyl-benzisoxasole-β-acetic acid, although the FeCl3 reaction makes it not impossible that it is 2-hydroxy-5-methylcinnamhydroxamic acid.

IT 861544-97-0P, Melilotic acid, β-carbamido-3-methyl-
861589-95-9P, Melilotic acid, β-carbamido-5-methyl-
RL: PREP (Preparation)
(preparation of)

RN 861544-97-0 CAPLUS

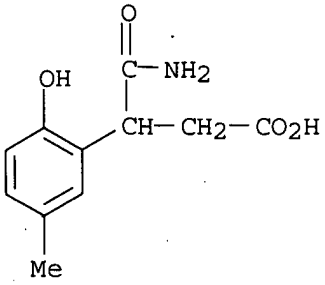
CN Melilotic acid, β-carbamido-3-methyl- (1CI) (CA INDEX NAME)



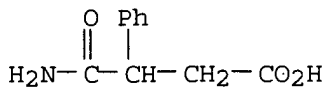
RN 861589-95-9 CAPLUS

CN Melilotic acid, β-carbamido-5-methyl- (1CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT



L17 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1908:10697 CAPLUS
DN 2:10697
OREF 2:2382b-d
TI On the Amic Acids of Phenylsuccinic Acid
AU Anschutz, Richard; Walter, Paul
CS Univ. Bonn.
SO Ann. (1908), 361, 73-8
DT Journal
LA Unavailable
AB It had been shown that NH3 and phenylsuccinic anhydride reacted so that the NH2 was added to the weaker carboxyl (Ibid., 354, 117; C. A., 1907, 2702). Luttgen (Dissertation, Bonn, 1899) found the opposite. Ethyl phenylcyanpropionate and concentrate H2SO4 yielded ethyl phenylsuccinamate, m. 173° (Luttgen, m. 167°. The product obtained from NH3 and phenylsuccinic anhydride was converted into the Ag salt and with EtI yielded a small amount of α-phenylsuccinamic-β-ethylester, m. 173°, but as main product the isomeric β-amicα-ester, m. 148-50°. The methyl esters were prepared similarly and separated quantitatively by ether. α-Amide-β-methyl ester, m. 145°; β-amide-α-methyl ester, m. 119°. The main product formed therefore contains the NH2 on the weaker carboxyl although at the same time some of the isomer is obtained.
IT 712-56-1, Succinamic acid, β-phenyl-
(and esters)
RN 712-56-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1907:11153 CAPLUS
DN 1:11153
OREF 1:2702f-i,2703a-i
TI On the Ester and Amide Acids of Phenylsuccinic Acid
AU Anschutz, Richard
CS Univ. Bonn
SO Ann. (1907), 354, 117-51
DT Journal
LA Unavailable
OS CASREACT 1:11153
GI For diagram(s), see printed CA Issue.
AB The effect of the negative phenyl group on the acidity of the carboxyl

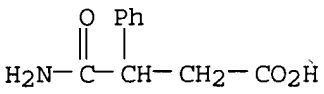
group attached to the same carbon atom of phenylsuccinic acid was studied. The chlorides of the two phenyl succinic acid monomethyl esters with benzene and aluminium chloride yielded the methyl ester of desylacetic acid in the one case and of phenylphenacylacetic acid in the other, fixing the structures of the two mono-esters. These were also determined by syntheses from benzalmalonic ester by adding hydrocyanic acid saponifying the cyanogen compound and then hydrolyzing to form the α-amide-β-acid, and by hydrolyzing the cyanogen compound directly to the β-ester-α-acid. Ammonia with amines unites with phenylsuccinic acid anhydride, the amidyl group combining with the carbonyl of the weaker (β) carboxyl group. On esterification of the anhydride, 75% β-ester-α-acid and 25% α-ester-β-acid were formed. Partial saponification of the neutral methyl ester yielded the weaker ester acid (α-ester-β-acid). Experimental. A. THE TRANSFORMATION OF PHENYLCYANPROPIONIC ACID AND ITS METHYL ESTER INTO PHENYLSUCCINIC-α-AMIDE-β-ACID AND PHENYLSUCCINIC-β-METHYLESTER-α-ACID (with Paul Walter). Phenylcyanpropionic acid, m. 150°, prepared from benzalmalonic acid ethyl ester (Bredt and Kallen, Ibid., 293, 345) with concentrated H2SO4 at the ordinary temperature for 12-hours gave phenylsuccinic-α-amide-β-acid. C8H6.CH(CONH2)CH3.CO2H, m. 158-159°. Ag salt. Methyl benzalmalonate, b16 170-171°, m. 44-45°, with potassium cyanide in methyl alcoholic solution yielded phenylcyanpropionic acid methyl ester, m. 55°, from which the methyl ester of the α-amide-β-acid, m. 145°, was prepared. The same ester was obtained from the above silver salt and methyl iodide. This ester when treated with sodium nitrate in a cold solution containing strong H2SO4 yielded phenylsuccinic-β-methyl ester-α-acid, C6H5.CH(CO2H).CH2.CO2CH3, m. 92°, identical with the main product obtained by the action of methyl alcohol on phenylsuccinic acid anhydride. B. THE FORMATION OF THEPHENYLSUCCINIC-METHYL ESTER ACIDS AND THEIR CHLORIDES (with Carl Hahn and Paul Walter). Phenylsuccinic acid, m. 167°, was prepared, starting with benzyl chloride, by methods already described (Ber., 14, 1645; 19, 1949; 24, 1877; Ann., 219, 30; 258, 74). Phenylsuccinylchloride, b12 150-151°, C6H5.CH(COCl).CH2.COCl. Phenylsuccinic acid anhydride, b12 191-192°. Dimethyl ester, b12 160-162°, m. 57-58°, on partial saponification with the calculated amount of alcoholic potash yielded the α-methyl ester-β-acid, m. 102-103°, C6H5CH(CO2CH3).CH2CO2H, whose constitution follows from the fact of the isomeric β-ester-α-acid, m. 92°, having the other structure as proved before. (Part A). Methyl alcohol and the anhydride yielded 25% α-ester-β-acid and 75% β-ester-α-acid. The chlorides of the ester acids were not obtained pure. C. THE ISOMERIC PHENYLSUCCINAMIDE-ANILIDE, p-TOLUIDINE-,AND PIPERIDIDE-ACIDS (with Carl Hahn and Paul Walter). The action of ammonia on the anhydride produced the β-amide-α-acid, m. 144-145°, C6H5.CH(CO2H).CH2CONH2. Ag salt Methyl ester, m. 119°, with nitrous acid yielded the α-ester-β-acid, m. 102°. This amide acid was insoluble in ether, the α-amide-β-acid, m. 119°, easily soluble. By this means the mixture obtained by the action of ammonia on the acid chloride was separated. Similarly the following substances were prepared. Phenylsuccinic-β-anilide-α-acid, C6H5.CH.(CO2H).CH2CONHC4H5, m. 169-170°. Ag salt. Methyl ester, m. 149°. α-Anilide-β-acid, C6H5.CH(CONHC2H3).CH3.CO2H, m. 175°. Methyl ester, m. 96°. From either anilide acid on heating with acetyl chloride, phenylsuccinanil, C6H5.CH.CO.N(C6H5).CO.CH7, m. 138°. was prepared. The anilide acid chloride and aniline yielded the dianilide, C3H3.CH(CONHC2H5).CH2.CONHC6H3 m. 222°. Phenylsuccinic-β-p-toluidide-α-acid, m. 168-169°, C6H5.CH(CO2H).CH2.CONH(4) C4H4(2)CH3. Ag salt. Methyl ester, m.

CAS ONLINE PRINTOUT

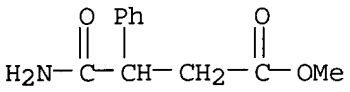
118°. α-p-Toluidide-β-acid, m. 175°. Methyl ester, m. 118° (same m. as the isomer, but mixed m. 105°). Phenylsuccin-p-tolil,C6H3.CH.CO.NH(4)C6H4(1)CH6.CO.CH2, m. 139°. Phenylsuccinic-β-piperidide-α-acid, C6H3.CH(CO2H).CH2.CONC6H3. m. 95°. Ag. salt. Methyl ester m. 109°, α-Piperidide-β-acid, m. 165° Methyl ester, m. 97°. D. SYNTHESIS OF DESYLACETIC ACID AND PHENYLPHENACYLACETIC ACID FROM PHENYLSUCCINIC ACID (with Paul Walter). By the action of benzene and aluminium chloride on phenylsuccinic-β-methyl ester α-acid chloride, desylacetic acid methyl ester (or β-phenyl-β-benzoyl-propionic acid methyl ester), C6H5.CH(COC6H5).CH2.CO2CH5, m. 49° (Ber., 21, 1305, 1349) was obtained; free acid, m. 162°. The same reaction with the β-ester-α-acid chloride produced phenylphenacylacetic acid methyl ester (or α-phenyl-β-benzoylpropionic acid methyl ester, m. 104°, C6H6CH.(CO2CH5).CH2.COC6H5 (Ann., 284, 3)); free acid, m. 153°. This reaction also proved the structures of the two ester acids of phenylsuccinic acid. The results obtained with mesaconic and phenylsuccinic acids are summoned up at the close. Partial esterification yielded both ester acids but in different amounts. Partial saponification of the neutral esters replaced the alkyl group of the weaker carboxyl by hydrogen. The melting points of the isomeric derivatives of the ester acids of phenylsuccinic acid are given in a table.

IT 712-56-1P, Succinamic acid, β-phenyl- 859961-47-0P, Succinamic acid, β-phenyl-, Me ester
RL: PREP (Preparation)
(preparation of)

RN 712-56-1 CAPLUS
CN Benzenepropanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)



RN 859961-47-0 CAPLUS
CN Succinamic acid, β-phenyl-, Me ester (1CI) (CA INDEX NAME)



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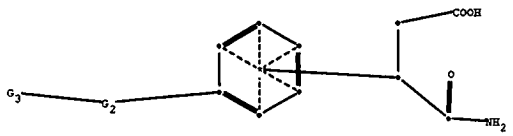

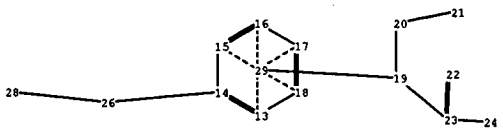

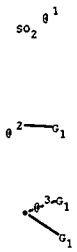

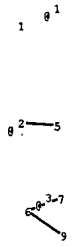

chain nodes :
1 2 5 6 7 9 19 20 21 22 23 24 26 28
ring nodes :
13 14 15 16 17 18
chain bonds :
2-5 6-7 6-9 14-26 19-23 19-20 20-21 22-23 23-24 26-28
ring bonds :
13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
2-5 6-7 6-9 14-26 22-23 23-24 26-28
exact bonds :
19-23 19-20 20-21
normalized bonds :
13-14 13-18 14-15 15-16 16-17 17-18

G1:H,CH3,CH2,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cy

G2:CH2,O,S,[*1],[*2],[*3]

G3:Cb,Cy,Hy,Ak

Match level :

1:CLASS2:CLASS5:CLASS6:CLASS7:CLASS9:CLASS13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS20:CLASS21:CLASS22:CLASS23:CLASS24:CLASS26:CLASS28:CLASS29:Atom

10/569812 MMP - UPDATED SEARCH REG NUMBERS

```
=> s 845786-15-4/RN or 845786-16-5/RN or 845786-17-6/RN or  845786-18-7/RN or
845786-19-8/RN or 845786-20-1/RN or 845786-21-2/RN or 845786-22-3/RN or
845786-23-4/RN or 845786-24-5/RN or  845786-25-6/RN or  845786-26-7/RN or
845786-27-8/rn
             1 845786-15-4/RN
             1 845786-16-5/RN
             1 845786-17-6/RN
             1 845786-18-7/RN
             1 845786-19-8/RN
             1 845786-20-1/RN
             1 845786-21-2/RN
             1 845786-22-3/RN
             1 845786-23-4/RN
             1 845786-24-5/RN
             1 845786-25-6/RN
             1 845786-26-7/RN
             1 845786-27-8/RN
L12         13 845786-15-4/RN OR 845786-16-5/RN OR 845786-17-6/RN OR  845786-18
               -7/RN OR 845786-19-8/RN OR 845786-20-1/RN OR 845786-21-2/RN OR
              845786-22-3/RN OR 845786-23-4/RN OR 845786-24-5/RN OR  845786-25-
              6/RN OR  845786-26-7/RN OR  845786-27-8/RN

=> d l12 1-13 ide

L12  ANSWER 1 OF 13  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   845786-27-8  REGISTRY
ED   Entered STN:  17 Mar 2005
CN   Benzeneacetic acid, α-(2-amino-2-oxoethyl)-4-(2-cyclohexylethoxy)-
     (9CI)  (CA INDEX NAME)
MF   C18 H25 N O4
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT, USPATFULL
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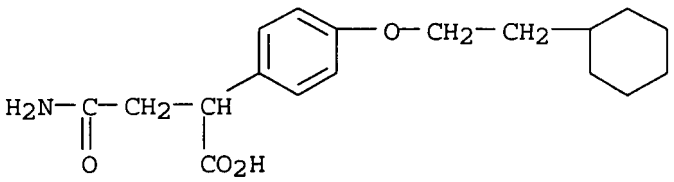

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               1 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12  ANSWER 2 OF 13  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   845786-26-7  REGISTRY
ED   Entered STN:  17 Mar 2005
CN   [1,1'-Biphenyl]-4-acetic acid, α-(2-amino-2-oxoethyl)-4'-methoxy-
     (9CI)  (CA INDEX NAME)
MF   C17 H17 N O4
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT, USPATFULL
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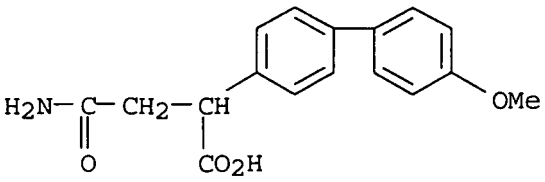
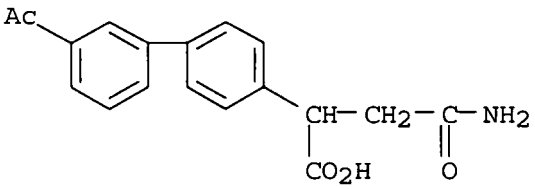


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

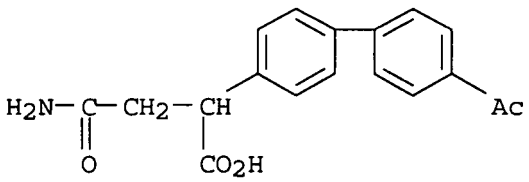
L12 ANSWER 3 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-25-6 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-acetic acid, 3'-acetyl-α-(2-amino-2-oxoethyl)-
(9CI) (CA INDEX NAME)
MF C18 H17 N O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

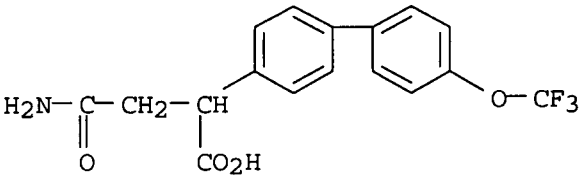
L12 ANSWER 4 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-24-5 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-acetic acid, 4'-acetyl-α-(2-amino-2-oxoethyl)-
(9CI) (CA INDEX NAME)
MF C18 H17 N O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

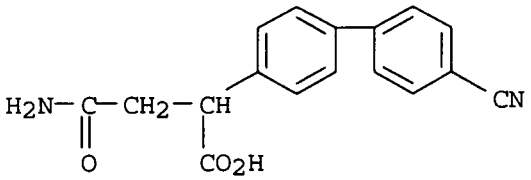
L12 ANSWER 5 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-23-4 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-acetic acid, α-(2-amino-2-oxoethyl)-4'-(trifluoromethoxy)- (9CI) (CA INDEX NAME)
MF C17 H14 F3 N O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 6 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-22-3 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-acetic acid, α-(2-amino-2-oxoethyl)-4'-cyano- (9CI) (CA INDEX NAME)
MF C17 H14 N2 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

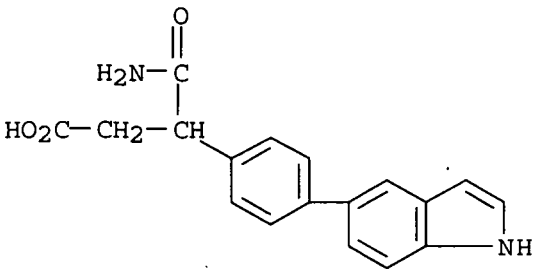


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 7 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-21-2 REGISTRY
ED Entered STN: 17 Mar 2005
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-(1H-indol-5-yl)- (9CI) (CA INDEX NAME)

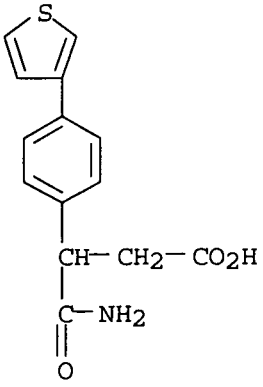
MF C18 H16 N2 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 8 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-20-1 REGISTRY
ED Entered STN: 17 Mar 2005
CN Benzenepropanoic acid, β-(aminocarbonyl)-4-(3-thienyl)- (9CI) (CA INDEX NAME)
MF C14 H13 N O3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

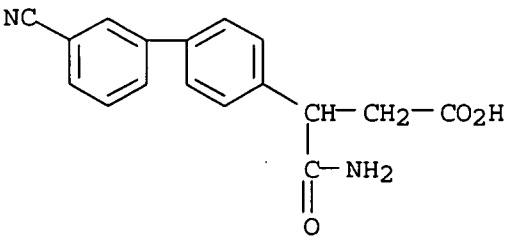


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 9 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-19-8 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-propanoic acid, β-(aminocarbonyl)-3'-cyano- (9CI) (CA INDEX NAME)

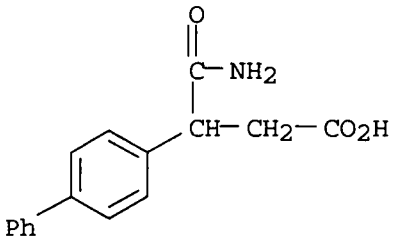
MF C17 H14 N2 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

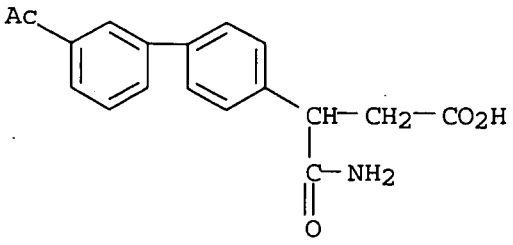
L12 ANSWER 10 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-18-7 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-propanoic acid, β-(aminocarbonyl)- (9CI) (CA INDEX NAME)
MF C16 H15 N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

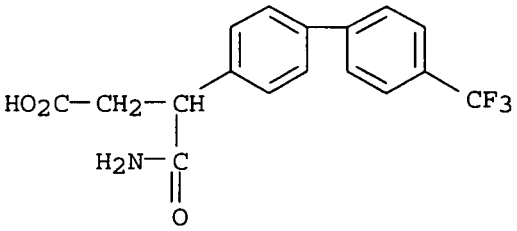
L12 ANSWER 11 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-17-6 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-propanoic acid, 3'-acetyl-β-(aminocarbonyl)- (9CI) (CA INDEX NAME)
MF C18 H17 N O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 12 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-16-5 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-propanoic acid, β-(aminocarbonyl)-4'-(trifluoromethyl)- (9CI) (CA INDEX NAME)
MF C17 H14 F3 N O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 13 OF 13 REGISTRY COPYRIGHT 2007 ACS on STN
RN 845786-15-4 REGISTRY
ED Entered STN: 17 Mar 2005
CN [1,1'-Biphenyl]-4-propanoic acid, β-(aminocarbonyl)-4'-cyano- (9CI) (CA INDEX NAME)
MF C17 H14 N2 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL